

Supplementary data for

Assessing ligand selectivity of sphingosine kinases with molecular dynamics and MM-PBSA binding free energy calculations

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Figure S1.Line Plot of the residue score

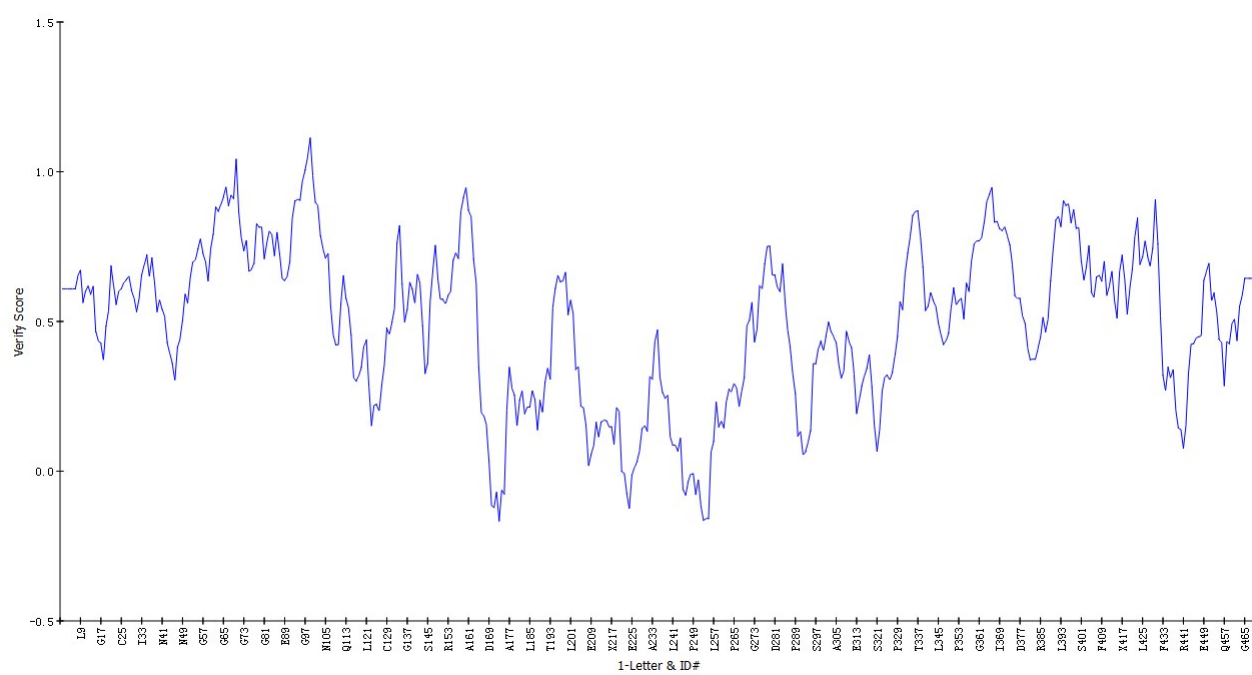
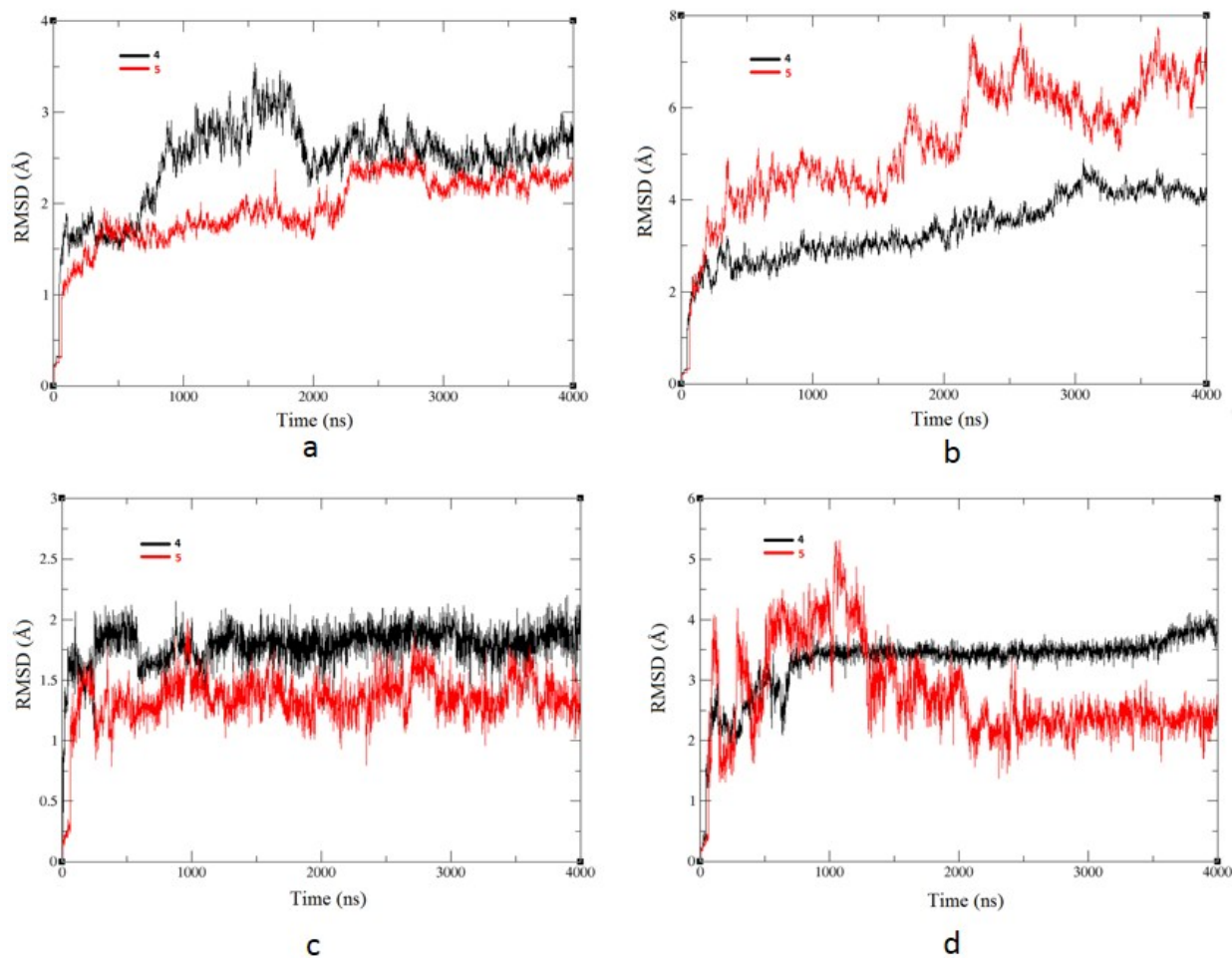


Figure S2 RMSDs of additional study



(a) RMSD of backbone atoms of protein in SK1 complexes; (b) RMSDs of backbone atoms of protein in SK2 complexes; (c) RMSDs of ligands in SK1 complexes; (d) RMSDs of ligands in SK2 complexes